

Properties of the perturbative expansion around the mode-coupling dynamical transition in glasses

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In this letter we show how to perform a systematic perturbative approach for the mode-coupling theory. The results coincide with those obtained via the replica approach. The upper critical dimension turns out to be always 8 and the correlations have a double pole in momentum space in perturbations theory. Non-perturbative effects are found to be very important. We suggest a possible framework to compute these effects.

In the mean field theory of glasses there are two transitions, the dynamical-replica transition, that corresponds to the mode-coupling transition in the dynamics and happens at a temperature T_c , and a thermodynamical transition (the Kauzmann transition) that happens at a lower temperature T_K [1, 2]. The dynamical-replica transition can be identified by looking at equilibrium properties of the system, i.e. its landscape; it corresponds to the formation of local minima in the free energy and it is usually studied using replicas [3–5]. The mode-coupling transition is defined by the dynamical properties of the system. The two transitions are related as far as in the mean field approximation the time needed to escape from a local minimum of the free energy is infinite.

This picture is exact in many solvable models. However it should be modified in the real world, where the mean field approximation is no more exact. In this letter we do not address the fate of the thermodynamical transition and we concentrate our attention on the dynamical mode-coupling transition.

It is quite evident that in short range systems there is no dynamical transition, exactly for the same reasons for which there are no infinite lifetime metastable states. However if we neglect the so-called “activated” process, the dynamical transition is present. Moreover there is a very large amount of experimental and numerical data that are well fitted by the predictions of the mode-coupling theory, so that it is certain interesting to try to understand which is the critical behaviour associated to the mode-coupling transition.

In this letter we present a computation of the upper critical dimensions and of the critical properties of the dynamical mode-coupling transition: in the dynamics we consider only the mutual dependence of quantities that do not depend explicitly on the time, i.e. time has been eliminated parametrically as it happens in the generalized fluctuation dissipation relations [6, 7]. We will firstly present the results in the framework of the equilibrium replica approach and we will later show how the same results hold for the mode-coupling transition.

The critical behaviour at the dynamical transition stems from the presence of dynamical heterogeneities [8–

13]. In the dynamics these heterogeneities are related to the presence of correlated movements of cooperatively rearranging regions [14] that have been observed both above and below the critical region around T_c . We are interested in getting precise predictions on the properties of dynamical heterogeneities.

Let us start with the basic definitions. Given two configurations of the coordinates (that we label with σ and τ), we indicate with $q_{\sigma,\tau}(x)$ the similarity (overlap) of the two configurations in the region of space around the point x (many different definitions are possible). Usually q is equal to one for identical configurations and it takes a small value for uncorrelated configurations [10, 15–17]. For example we can take $q_{\sigma,\tau}(x)$ to be one if a region around x of size a [31] has the same particle content in the configurations σ and τ ; otherwise $q_{\sigma,\tau}(x) = 0$, if the particle content is different.

Let us consider the case where σ is an equilibrium configuration of the system and $\tau(t)$ is a configuration obtained using some dynamics at time t starting from the σ configuration (i.e. $\tau(0) = \sigma$). If the dynamics is non-deterministic, the configuration $\tau(t)$ will depend also on some extra random variables η . For simplicity of notation we will not indicate the dependence of $\tau(t)$ on η , unless we need it in an explicit way. We can define

$$C(t) = \overline{q_{\sigma}(x, t)} \text{ where } q_{\sigma}(x, t) \equiv \langle q_{\sigma, \tau(t)}(x) \rangle. \quad (1)$$

Here the overline denotes the average over the Boltzmann distribution of the initial configuration (σ) and the angular brackets the average over η . $C(t)$ is the usual equal point (smeared over a region of size a) density-density correlation. Approaching the dynamical transition, $C(t)$ will decay slower and slower, and will also develop a plateau (as function of $\ln(t)$) at the value C_P . This plateau becomes infinitely long at the mode-coupling temperature; below the mode-coupling temperature, neglecting *activated processes*, the correlation does not decay any more, i.e. $\lim_{t \rightarrow \infty} C(t) \equiv C_{\infty} > C_P > 0$.

For the study of dynamical heterogeneities it is usual to consider a dynamical susceptibility $\chi_4(t)$ defined as

$$V\chi_4(t) = \overline{Q_{\sigma}(t)^2} - \overline{Q_{\sigma}(t)}^2 = \overline{(Q_{\sigma}(t) - C(t))^2}, \quad (2)$$

where V is the volume of the system and $Q_\sigma(t)$ is the space integral of $q_\sigma(x, t)$. The quantity $\chi_4(t)$ is a measure of the differences that are observed during the evolution from region to region [8–13]. In a similar fashion we can define the time dependent correlation function

$$G_4(x - y, t) = \overline{q_\sigma(x, t)q_\sigma(y, t)} - C(t)^2. \quad (3)$$

The explicit time dependence is quite a complex problem that we do not address in this letter; different dynamical exponents are involved and they are known to be not universal (at least in the mean field approximation). We will consider here only relations where the time is not explicitly presents, as the dependence of χ_4 on C , that can be obtained by eliminating the time parametrically, e.g. by plotting $\chi_4(t)$ versus $C(t)$ exactly in the same way as for the fluctuation dissipation relations. A particular example of a time independent quantity is χ_4^* , that is defined as the maximum of $\chi_4(t)$ (that happens at time t^*) (the corresponding correlation will be denoted by $G_4^*(x)$). Analogously we define a C -dependent correlation function $G_4(x - y|C)$ as follows

$$G_4(x - y|C(t)) = G_4(x - y, t). \quad (4)$$

We are interested in the universal properties of the previous quantities when we approach the dynamical transition. We denote by ϵ the distance in temperature from the dynamical transition and we indicate from here on the dependence on ϵ . We are interested in the behaviour in the double scaling limit $\epsilon \rightarrow 0$ and $C \rightarrow C_P$. Within mean field theory, the susceptibility $\chi_4(C_P, \epsilon)$ is divergent when $\epsilon \rightarrow 0$ from above [32]. Given the obvious relations $\chi_4^*(\epsilon) = \int G_4^*(x, \epsilon) dx$ the divergence of $\chi_4^*(\epsilon)$ implies the existence of a divergent correlation length $\xi(\epsilon)$. In the same way as in standard phase transitions, we expect the following scaling laws

$$\chi_4^*(\epsilon) \propto \epsilon^{-\gamma}, \quad \tilde{G}_4^*(k, \epsilon) = \chi_4^*(\epsilon) \tilde{g}_4(k\xi(\epsilon)), \quad \xi(\epsilon) \propto \epsilon^{-\nu}, \quad (5)$$

where $\tilde{G}_4^*(k, \epsilon)$ is the Fourier transform of $G_4^*(x, \epsilon)$.

What is the replica counterpart of this behaviour? In the replica approach [5] we consider two replicas σ and τ . We denote by $H(\sigma)$ the original Hamiltonian, while the Hamiltonian of the τ system is

$$H(\tau) - hQ_{\sigma, \tau}. \quad (6)$$

The thermal averages are taken first with respect to the τ variables and later with respect to σ variables. The dynamical phase transition is defined by the behaviour of $q_0(\epsilon) \equiv \lim_{h \rightarrow 0^+} q(\epsilon, h)$. For $\epsilon > 0$ we should have $q_0 = q_{bulk}$, i.e. a small value usually temperature independent; at $\epsilon = 0$ we should have $q_0(0) = C_P$ and for $\epsilon < 0$ we should have $q_0(\epsilon) > C_P$. This behaviour is present in mean field model where metastable states do exist. It survives in the real world in the approximation where metastable states can be observed. In other words the

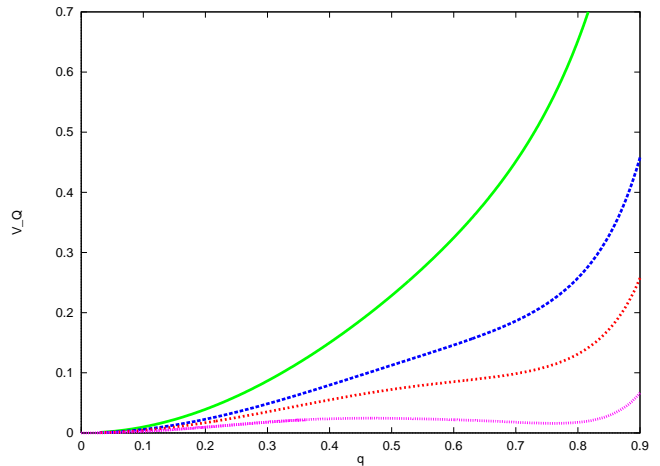


FIG. 1: A schematic view of the potential $W(q)$ computed at various temperatures, decreasing from above to below.

two replicas system (with the replica σ quenched respect to the replica τ) becomes critical at the same point where the dynamics display the mode-coupling singularity.

One can sharpen the physical picture by introducing a potential $W(q)$ defined as follows [2, 5, 18]. We consider an equilibrium configuration σ . We call $P_\sigma(q)$ the probability that another configuration τ has an overlap $q_{\sigma, \tau} = q$. We define

$$W(q) = - \lim_{V \rightarrow \infty} \frac{\ln(P_\sigma(q))}{V}. \quad (7)$$

With probability one when the volume V goes to infinity, the potential $W(q)$ does not depend on the reference configuration σ . In other words $P_\sigma(q) \approx \exp(-VW(q))$. By construction $W(q_{bulk}) = 0$ and the vanishing of the potential $W(q)$ for more than one q value is the distinctive characteristic of replica symmetry breaking (this should happen below an eventual thermodynamical glass transition). In other words we are considering an equilibrium configuration σ and we define by $W(q)$ the increase in the free energy density if we constrain an other equilibrium configuration τ to stay at overlap q .

The behaviour of the potential in the mean field approximation is described in Fig. 1. The dynamical transition is characterized by the presence of an horizontal flex for the potential $W(q)$. Beyond the mean field approximation the Maxwell construction should hold and the non convex part of the potential disappear, but we will not consider this effect.

A standard assumption is that the behaviour in the dynamics mirrors the behaviour in the equilibrium properties of two replicas of the system. This assumption is usually accepted and there are partial proofs of its validity in perturbation theory (we will come later to this point by showing how to complete these proofs). Let us try to formulate this assumption in a sharp way.

In the same way as the time may be eliminated parametrically, also the forcing field h may be eliminated in

favor of the expectation value of the overlap (i.e. q) and all other physical variables can be expressed as function of q ; this is the usual Legendre transformation of statistical mechanics. Our assumption is that in the critical region ($\epsilon \rightarrow 0$ and $C \rightarrow C_P$) the quantities

$$\chi_4(\epsilon|q), \quad \Gamma_4(x-y, \epsilon|q), \quad (8)$$

computed *in perturbation theory* in the replica approach are the same as those computed in the mode-coupling theory (as function of C). This relation holds only in the region of q where the forcing field $h \approx 0$.

Let us start the perturbative computation in the replica approach. The computations in the mode-coupling approach will be rather similar. It is quite clear from Fig. 1 that changing the temperature there is a critical point. Our task is to compute the critical properties using the standard renormalization group tools. We want to determine the critical exponents γ and ν and the scaling function $g_4(x/\xi)$, that according to the previous assumption are in the same perturbative universality class in the mode-coupling theory and in the replica approach. Let us discuss for the moment only the region below the dynamical temperature, i.e. $\epsilon < 0$, since this region is very well defined in the perturbative expansion.

In high dimensions the correlation function is just given by the mean field result [12, 19, 20]

$$\tilde{G}_4(k, \epsilon) = \frac{1}{(|\epsilon|^{1/2} + k^2)^2}, \quad (9)$$

thus leading to the following mean field exponents

$$\nu = \frac{1}{4} \quad \gamma = 1. \quad (10)$$

As we will see, there is a crucial difference among the double pole behaviour that we find to be valid in the general case and the single pole behavior. Notice that the double pole form in Eq.(9) is at variance with the single pole behavior predicted in [19, 20], if no local conservation laws are present. The reasons for this discrepancy will be discussed later, when we confirm the presence of a double pole by a dynamical analysis.

In order to compute the critical exponents of the dynamical transition we will start from the perturbation theory around the mean field theory. We will consider the most divergent diagrams near the critical point and we will identify the universality class of the problem. In this context we do not see that the critical point is in the metastable phase because this would be a non-perturbative effect.

This computation can be done within the replica method of [5] assuming a universal cubic effective replica action close to the inflection point of $W(q)$ for $\epsilon \rightarrow 0$. For disordered systems like Potts model, however, this model should be in the same universality class of structural glasses as far the dynamical transition is concerned.

We can define two correlations functions

$$\begin{aligned} G_0(x) &= \overline{\langle q_{\sigma,\tau}(x) \rangle \langle q_{\sigma,\tau}(0) \rangle} - \overline{\langle q_{\sigma,\tau}(0) \rangle}^2, \\ G_1(x) &= \overline{\langle q_{\sigma,\tau}(x) q_{\sigma,\tau}(0) \rangle} - \overline{\langle q_{\sigma,\tau}(x) \rangle \langle q_{\sigma,\tau}(0) \rangle}, \end{aligned} \quad (11)$$

where the overline denotes the average over the σ 's and $\langle \cdot \rangle$ the average over the τ 's.

In the case of a fluid with only one type of particles, $q_{\sigma,\tau}(x)$ can be written as $\sigma(x)\tau(x)$ (where $\sigma(x)$ and $\tau(x)$ are smeared densities around the point x) and the previous equations become

$$\begin{aligned} G_0(x) &= \overline{\langle \tau(x) \rangle \langle \tau(0) \rangle \sigma(x) \sigma(0)} - \overline{\langle \tau(0) \rangle \sigma(0)}^2, \\ G_1(x) &= \overline{\langle \tau(x) \tau(0) \rangle_c \sigma(x) \sigma(0)}. \end{aligned} \quad (12)$$

One finds that near the critical point (neglecting loops)

$$\tilde{G}_0(k, \epsilon) = \frac{1}{(\epsilon^{1/2} + k^2)^2}, \quad \tilde{G}_1(k, \epsilon) = \frac{1}{\epsilon^{1/2} + k^2}. \quad (13)$$

In order to compute the loop corrections one must use a precise replica setting. In the approach presented here, there is an annoying asymmetry among the replica σ and the replica τ . In the replica approach it corresponds to take one privileged replica σ and n replicas of type τ and sending the value of n to zero. It is known that a partially equivalent formalism consists in using m replicas that are constrained to be at overlap q and take the limit where m goes to one. In this different formulation we have a symmetry Z_m in the limit $m \rightarrow 1$ and it may be more convenient to use [22]. We checked that the two formulations are equivalent near the stationary point and for simplicity we present the analysis in this second formalism. A detailed discussion of this point will be presented elsewhere [23].

The diagrammatics is the same of an usual ϕ^3 theory with two differences [12, 21]: A) some of the propagators have a single pole, others have double poles; B) the multiplicity of the diagrams have to be computed in the limit where m goes to one and some diagrams give zero contribution in this limit.

One should do a careful analysis: at the end of a long analysis [23] we find that many diagrams give zero contribution and the dimension where the perturbative corrections are divergent is 8 [33]. Moreover the diagrams are the same of those for lattice animals, with the difference that here the effective coupling constant is positive (for lattice animals is negative) [24–26]. The value 8 for the upper critical dimension may provide an explanation for many of the anomalies found in [27].

What happens below (and near) 8 dimensions? The situation is quite puzzling: the renormalization group pushes the coupling constant g^2 toward a large value and there is no perturbative fixed point that we can analyze. Moreover the terms in the perturbation theory have all positive sign and therefore it is not easy to estimate the sum. This result is not so disturbing. Metastable states have finite life time, the free-energy acquires an imaginary

part that pushes the singularity in the complex plane; in the same way the coupling constant takes an imaginary part. Although the bare coupling is real, the fixed point may correspond to an imaginary coupling constant. One could argue that asymptotically the exponent are like those of lattice animals for the complex singularity.

However the previous conclusion may be too hasty. Using the same arguments of [24–26] one finds that the sum of the leading diagrams is related to the solution of the stochastic differential equation governing the local fluctuations of the overlap $\phi(x) = q(x) - q$ (being q the space average of $q(x)$)

$$-\Delta\phi_\omega(x) + A + \epsilon\phi_\omega(x) + g\phi_\omega(x)^2 = \omega(x) \quad (14)$$

where $\omega(x)$ is a Gaussian short range noise, that is $\omega(x)\omega(y) = \delta(x-y)$. A and g are smooth functions of the temperature and they are chosen in such a way to implement the condition $\overline{\phi_\omega} = 0$. The two propagators are given by the relations

$$\begin{aligned} G_0(x) &= \overline{\phi_\omega(x)\phi_\omega(0)}, \\ G_1(x) &= \overline{\phi_\omega(x)\omega(0)} = \left(\frac{1}{-\Delta + \epsilon + 2g\phi} \right)_{x,0}, \end{aligned} \quad (15)$$

where the last equality follows from integration by part (and it is correct only in case the solution to the stochastic differential equation is unique).

Neglecting technicalities, the physics is quite clear. The choice of the variables σ (i.e. the initial conditions in the dynamics) induce point dependent shift of the critical temperature and the effects of these fluctuations is the dominant one.

One may wonder if there is a direct role of $G_1(x)$ in the dynamics. A suggestion is the following. Let us consider a theory where the microscopic evolution equations for the particle have a stochastic nature. In this case the overlap $q_{\sigma,\tau}(x)$ will be a function of both the time t and of the noise $\eta(x,t)$ and it will be denoted by $q_{\sigma,\eta}(x,t)$. We can define a different dynamical susceptibility:

$$V_{\chi 22}(t) = \overline{\langle Q_{\sigma,\eta}(t)^2 \rangle} - \overline{\langle Q_{\sigma,\eta}(t) \rangle^2}, \quad (16)$$

and the corresponding correlation $G_{22}(x,t)$, where the overline denotes the average over initial conditions and angular brackets average over η [34]. One could argue that in the region of time where $C(t)$ is near to (and above) the plateaux, $G_{22}(x,t)$ should behave as $G_1(x)$. On the other hand in the region where $C(t)$ is small, the behaviour of $G_{22}(x,t)$ and $G_4(x,t)$ should be similar.

The whole analysis can be redone in the dynamical approach where one takes care in an explicit way the dependence of the correlations on the initial configuration (a fact that was neglected in [19]). The computations can be done in a neat way within the Martin-Siggia-Rose (MSR) formalism of equilibrium dynamics using a universal cubic dynamical action close to the mode-coupling transition. Detailed computations shows that taking care

of the correlations of the initial configuration with the evolving configurations one recovers the same result of the replica formalism. An explicit isomorphism of the two approaches can be shown to be present: the relevant computations will be presented in [23].

Let us come back to the replica approach and let us consider in more detail the stochastic differential equation (14) that is the resummation of the leading perturbative contributions. We are interested to study it in a non-perturbative way.

It is well known that in perturbation theory the solution of the stochastic differential equation is unique and that there is a hidden supersymmetry [24–26]. The supersymmetry relates the two propagators and gives

$$G_1(x) \propto \frac{1}{x} \frac{\partial G_0(x)}{\partial x}. \quad (17)$$

This supersymmetric relation is at the origin of the *dimensional reduction*: the critical exponents of lattice animals problem in dimensions D are the same of those of the Ising model near the Lee-Yang singularity in dimension $D-2$.

However in presence of multiple solutions (as e.g. for the Random Field Ising Model) everything becomes more complex (multiple solutions cannot be seen in perturbation theory so that this problem does not affect the perturbative analysis that we have presented above). Supersymmetry and dimensional reduction are only valid if we average over all the solution with a sign depending on the parity of the corresponding Morse index: this weight is not the natural one from the physical viewpoint [24–26].

Which is the correct weight? If we stay within the replica formalism it is useful to consider the free energy

$$F[q]_\omega = \int dx \left(\frac{1}{2} \frac{\partial^2 q(x)}{\partial x^2} + W(q(x)) - \omega(x)q(x) \right). \quad (18)$$

Equation (14) can be written as $\delta F[q]_\omega / \delta q(x) = 0$. Now the natural choice would be to consider among the many solutions the one that minimize $F[q]_\omega$. On the other hand this choice is not natural in the dynamics where we would like to take the solution $q_M(x)$ that maximize $q(x)$. Indeed it can be proved [28] that there is a solution $q_M(x)$ such that $q_M(x) > q(x)$ for all x and for any possible solutions of the stochastic differential equation (this is a well known fact in the Random Field Ising Model [28]). In both cases dimensional reduction is no more valid and non-perturbative effects are present.

A neat formulation of the problem is the following: we introduce a fictitious time s and we write the following evolution equation:

$$\frac{\partial q(x,s)}{\partial s} = -\Delta q(x,s) + W'(q(x,s)) - \omega(x) \quad (19)$$

with the boundary conditions at time $s=0$ given by $q(x,0) = 1$. In the region below T_c , where the equation

(14) has many solutions, the solution relevant for the dynamics is uniquely identified as

$$q_{\omega}^*(x) = \lim_{s \rightarrow \infty} q_{\omega}(x, s) . \quad (20)$$

We are near to the end of our journey. We still have to compute the critical exponent and the critical behaviour of the correlation of $q_h^*(x)$. Techniques introduced in [29] could be used to achieve this goal.

We remark that the fictitious time s in the equation (19) should not be identified with the real time: the dependence of $q(s)$ if we solve equation (19) is quite different from the behaviour of $q(t)$ in mode-coupling theory and there should be no confusion among the two variables. However one may make *en passant* the conjecture that, if we consider only reparametrization invariant quantities, the mode-coupling equations and eq. (19) stay in the same universality class: in other words, if in the mode-coupling theory we eliminate the real time t in favour of q and we write everything as function of q and in eq. (19) we eliminate the fictitious time s in favour of q , the dependence of the physical quantities on q should be the same near the critical point for the models. This conjecture is trivially valid if there is only one solution of equation (14). The point is to understand its correctness beyond perturbation theory

This conjecture may be generalized by introducing a more general evolution equation that can be used to compute the properties of reparametrization invariant quantities when activated processes are present below T_c :

$$\frac{\partial q(x, s)}{\partial s} = -\Delta q(x, s) + W'(q(x, s)) - \omega(x) + \eta(x, s) \quad (21)$$

where $\eta(x, s)$ is a thermal noise. The discussions of the consequences of these conjectures cannot be done here, however it has not escaped to how attention that eq. (21) can be used to explain the experimental results of [30].

Summarizing, we have clarified the predictions and the limitations of the perturbative expansions for the critical properties of glasses, finding an explicit mapping among the replica formalism and the mode-coupling approach in the framework of the MSR approach to the dynamics. We have also conjectured a mapping with a differential stochastic equations that should be valid beyond perturbation theory, whose interesting consequences should be studied in details.

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- [31] Typically the ratio of a with the inter-particle distance is taken to be smaller than 1 and not far from the Lindemann constant.
- [32] We implicitly assume that the maximum $\chi_4^*(\epsilon)$ happens in the critical region $C \approx C_P$.
- [33] The value 8 for the upper critical dimension was first suggested in [12]. Then the value 6 was found in [19], while only in some particular cases (i.e. in presence of locally conserved quantities) the value was suggested to be equal to 8 [20].
- [34] Notice the difference in the averaging procedure between the second addend in χ_{22} and the one in χ_4 .